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Effect of the size of calixarene macrocycle on the thermodynamic parameters of formation of inclusion compounds in guest vapor - Solid host systems

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Abstract

The influence of the calixarene macrocycle size on the thermodynamic parameters of inclusion formation in organic guest vapor - solid host systems was studied in the series of tert-butylcalix[4]arene (1), tert-butylcalix[6] arene (2), and tert-butylcalix[8]arene (3). For this purpose, sorption isotherms of a guest vapor by a solid host were determined using the static method of headspace GC analysis for the systems involving calixarenes 2 and 3 in addition to the earlier obtained data for calixarene 1. Besides, the stoichiometry and decomposition temperatures of saturated clathrates formed in these systems were determined using thermogravimetry. The compositions of some of these clathrates differ substantially from those of clathrates crystallized from a host solution in a liquid guest. For the most guests studied with the thermodynamic activity below 0.6, their uptake by calixarenes 1 - 3 changes in the series 2 < 1 < 3. As a whole, the trend for each particular parameter of clathrates of hosts 1 - 3 (stoichiometry, guest activity at 50% saturation of the host) with increasing the size of the calixarene macrocycle is specific for each guest studied. The results obtained are useful for the estimation of receptor properties of calixarenes in quartz microbalance sensors.

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Keywords

clathrates, guest - host inclusion compounds, headspace GC analysis, sorption isotherms, thermogravimetry